Artemisinic aldehyde

Inchi: InChI=1S/C15H22O/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)15(13)8-10/h8-9,11,13-15H,3-7
InchiKey: SVAPNGMAOHQQFJ-ZGKBOVNRSA-N
Formula: C15H22O
SMILES: C=C(C=O)C1CCC(C)C2CCC(C)=CC12
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	133.20	kJ/mol	Joback Method
hf	-196.28	kJ/mol	Joback Method
hfus	25.15	kJ/mol	Joback Method
hvap	55.96	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.760		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinpol	1675.00		NIST Webbook
ripol	2144.00		NIST Webbook
tb	613.18	K	Joback Method
tc	831.74	K	Joback Method
tf	311.69	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.42	J/mol×K	613.18	Joback Method
cpg	553.15	J/mol×K	649.61	Joback Method
cpg	573.52	J/mol×K	686.03	Joback Method
cpg	592.59	J/mol×K	722.46	Joback Method
cpg	610.41	J/mol×K	758.89	Joback Method
cpg	627.03	J/mol×K	795.31	Joback Method
cpg	642.51	J/mol×K	831.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R603779&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume